

Model

C. B. Das and S. Das Gupta

Physics Department, McGill University, 3600 University St., Montréal, Québec

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Abstract

For pedagogical reasons we compute the caloric curve for 11 particles in a 3^3 lattice. Monte-Carlo simulation can be avoided and exact results are obtained. There is no back-bending in the caloric curve and negative specific heat does not appear. We point out that the introduction of kinetic energy in the nuclear Lattice Gas Model modifies the results of the standard Lattice Gas Model in a profound way.

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I. INTRODUCTION

In a recent paper [1], we pointed out that microcanonical calculations in the Lattice Gas Model (LGM) with constant energy are no harder to implement than canonical calculations with constant temperature. We will call the first MLGM, and the second, CLGM. For practical cases at hand ($A \approx 100$ or 200), the calculations use Monte-Carlo simulations with Metropolis algorithm. We found that in LGM, as used in nuclear disintegration problems, there is no “backbending” in the caloric curve for systems as small as ^{84}Kr whether in microcanonical or canonical treatments. By “backbending” one means an “S” shape when energy is plotted along the y-axis and temperature along the x-axis. Since microcanonical treatments seem to lead to backbending for small systems (100 particles is small enough) in other models [2–4], our findings need some clarification. Motivated by this, we present here results for a very small system, 11 particles in 3^3 lattice. Here we can avoid Monte-Carlo samplings and do exact (though it still requires some numerical work which is easy) computations. The results are quite interesting and not only explain our previous findings but also shed light on several connections between microcanonical and canonical calculations.

II. THE MODEL SYSTEM

As our objective is solely pedagogical, we assume there is just one kind of particles (nucleons). We take the number of particles to be 11. The lattice space is 3^3 . This then implies a freeze-out density $0.41\rho_0$ which is somewhat higher than the freeze-out density used in lattice gas model calculations [5]. The nearest neighbour bonds are attractive: $\epsilon = -5.33\text{MeV}$ to get the nuclear matter binding energy correct.

The nuclear Lattice Gas Model which is denoted here by LGM is an extension of the standard textbook Lattice Gas Model as discussed, for example, in [6]. We denote the standard lattice gas model by SLGM. The difference is simple: in SLGM, the nucleons are frozen in their lattice sites. In LGM, dictated by the physics of the nuclear problem, they

are given momenta. In CLGM, these momenta are generated using a Maxwell-Boltzmann distribution. In MLGM, they are taken from a uniform distribution within a sphere in momentum space. The addition of kinetic energy, however, changes the caloric curve in an interesting and profound way. We will find it useful to discuss the caloric curves in both SLGM and LGM. Chronologically, it is easier to discuss SLGM first, then point out how LGM modifies the results. In both the models the key quantities are $G(27, 11, N_{nn}) \equiv g(N_{nn})$ = the number of configurations with N_{nn} nearest neighbour bonds for the case of 11 particles in 3^3 lattice sites. Once these are known both canonical and microcanonical calculations are readily done. The degeneracy factors are given in the small table. They can be obtained with little effort in this simple case.

N_{nn}	$g(N_{nn})$	N_{nn}	$g(N_{nn})$
0	462	9	2643624
1	888	10	1895907
2	8511	11	1051632
3	38128	12	481610
4	150030	13	174408
5	481368	14	50301
6	1171492	15	8984
7	2106504	16	1056
8	2772894	17	96

Table I: Degeneracy factors $g(N_{nn})$ with N_{nn} nearest neighbour bonds.

III. MICROCANONICAL TREATMENT OF SLGM

Instead of writing $g(N_{nn})$ we will find it convenient to write g as a function of E^* where E^* is the excitation energy. The degeneracy factor $g(E^*)$ as a function of $E^*/|\epsilon|$ is plotted in Fig. 1. The distribution is discrete but in Fig.1 we show it as a continuous distribution

and label the y-axis by $dN(E^*)/d|\epsilon|$. If one wants to define a temperature, the standard practice in the microcanonical model is to compute $\frac{\partial \ln \Omega(E^*)}{\partial(E^*)} \equiv \frac{1}{T}$ (see [7]). An inspection of Fig.1 shows that as a function of excitation energy the temperature will rise first, approach $+\infty$, will then switch towards $-\infty$ and as the excitation energy will further increase the temperature will approach 0 from the negative side. This happens because in SLGM there is an upper bound to energy. This is of course well-known for spin 1/2 systems in a magnetic field if the kinetic energy of the spin system is suppressed [7]. In nuclear shell model, for example, this will happen if one restricts oneself to limited shell model orbitals. This is well-known to practitioners [8].

The caloric curve in microcanonical SLGM is shown in Fig. 2. In plotting this curve we used degeneracies of successive discrete points in the excitation energy and divided by $|\epsilon|$ to get the temperature. Notice that in the positive side of the temperature there is no anomalous behaviour. If we plot E^* along the y-axis and T along the x-axis, there is a “giant” size backending at about half the excitation energy available to the system. But this is merely a reflection of the fact that the excitation energy available to the system is finite. This will drastically change in the nuclear LGM where availability of kinetic energy will remove the upper limit.

IV. CANONICAL TREATMENT OF SLGM

For canonical calculation, we pick a positive temperature: to get the caloric curve we compute $\langle E \rangle = \sum \epsilon N_{nn} \times g(N_{nn}) \exp(-\beta N_{nn} \epsilon) / \sum g(N_{nn}) \exp(-\beta N_{nn} \epsilon)$. Subtracting out the ground state energy we obtain the plot in Fig. 2. The same procedure can be used for negative temperature. Both are used in Fig. 2. The similarity between caloric curves calculated in the microcanonical and canonical models is obvious although there are quantitative differences.

V. MICROCANONICAL CALORIC CURVE IN NUCLEAR LGM

From SLGM we now turn to nuclear LGM which serves as a model for nuclear disassembly. This was the case presented in [1]. The excitation energy can come from two sources now: kinetic and potential. Consequently, we compute $\sum_i g(E_i^*)\rho_{kin}(E^* - E_i^*)$ where $g(E_i^*)$ is discrete and taken from the table and $\rho_{kin}(E_{kin})$ is taken to be the integral

$$\int \delta(E_{kin} - \sum p_i^2/2m) \Pi d^3 p_i = \frac{(\sqrt{\pi})^{3N}}{\Gamma(3N/2)} (2m)^{3N/2} E^{3N/2-1} \quad (5.1)$$

N in our chosen case is 11. Now there is no upper limit to E^* . In Fig. 3 we have plotted $\sum_i g(E_i^*)\rho_{kin}(E^* - E_i^*)$. The most important difference from Fig. 1 is that the negative temperature zone has completely disappeared. Thus the difference in the caloric curves obtained from SLGM and LGM will be profound.

There are two ways one can calculate the temperature in the microcanonical model. One is the standard formula : $\frac{1}{T} = \frac{\partial \ln \Omega(E^*)}{\partial E^*}$ where

$$\Omega(E^*) \propto \sum_i g(E_i^*)\rho_{kin}(E^* - E_i^*) \quad (5.2)$$

The other intuitive approach would be to make the following ansatz. Although we are talking of one system only, formally eq. (5.2) is similar to that of two systems characterised by g and ρ_{kin} which share energy with each other but are insulated from the rest of the universe so that the total energy E^* does not change. If the systems characterised by g and ρ are large then the sum above would be dominated by the largest term in the sum which is obtained when the temperature of each subsystem is the same, i.e., $\frac{\partial \ln g(E_i^*)}{\partial E_i^*} = \frac{\partial \ln \rho_{kin}(E_{kin})}{\partial E_{kin}}$. We now use $\frac{1}{T} = \frac{\partial \ln \rho_{kin}(E_{kin})}{\partial E_{kin}}$. This leads to $\langle T \rangle = \langle E_{kin} \rangle / (1.5N - 1)$. This $\langle T \rangle$ and the standard definition of T agree quite well as can be seen in Fig.4. Notice also there is no backbending in the microcanonical caloric curve. If one wants to use the microcanonical nuclear LGM for practical calculations with nucleon numbers about 100 or higher and also wants to obtain a value for temperature, getting the temperature from kinetic energy is the only easy option.

In Fig.4 we have also shown the caloric curve in nuclear LGM in the canonical model. This agrees with the microcanonical calculation quite well.

VI. A SADDLE-POINT CALCULATION

In the particular example (11 particles in 3^3 boxes in the nuclear LGM), one has exact expressions for microcanonical density of states. One can also compute numerically the canonical partition function. In nuclear physics one often has numerical values for canonical or grand canonical partition functions. The direct expression for the microcanonical density of state is usually intractable and in order to obtain a value one uses the saddle-point approximation [9,10]. We can use the nuclear LGM to test the accuracy of the saddle-point approximation since here both the microcanonical density of state and the canonical partition function are directly calculable. The microcanonical density of states and the canonical partition function are related by $Q(\beta) = \int \exp(-\beta E) \rho(E) dE$. The inverse transformation is $\rho(E) = \exp(\beta_0 E) \frac{1}{2\pi} \int \exp(i\beta E) Q(\beta_0 + i\beta) d\beta$. The saddle-point approximation for this integral leads to

$$\rho(E) \approx \frac{\exp[\beta_0 E + \ln Q(\beta_0)]}{\sqrt{2\pi(< E^2 > - < E >^2)}} \quad (6.1)$$

where the value of β_0 is so chosen that at this value $< E > = E$. The saddle-point approximation for the density of states is also compared to the exact density of state in Fig.3. Except for low excitation energies, the saddle-point approximation is seen to be excellent.

VII. SUMMARY

We performed an exact microcanonical calculation of the caloric curve of 11 particles in a 3^3 lattice. The caloric curve does not have a backbending which means there was no negative specific heat in this model for 11 particles. We then conclude that the phenomenon of backbending can be quite model dependent.

VIII. ACKNOWLEDGMENTS

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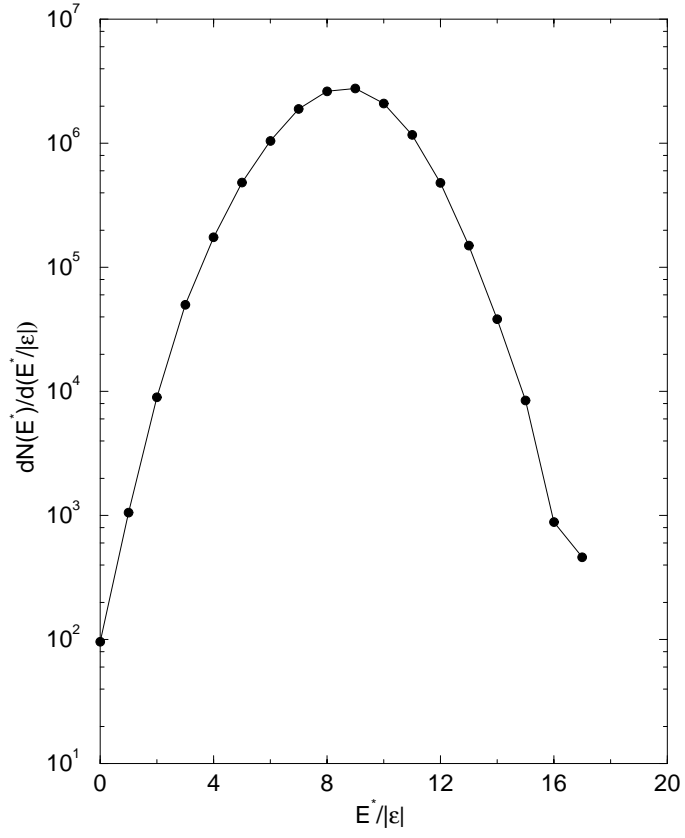


Fig. 1: The density of states in the standard lattice gas model. This can be directly obtained from the table remembering that $N_{nn} = 17$ defines the ground state.

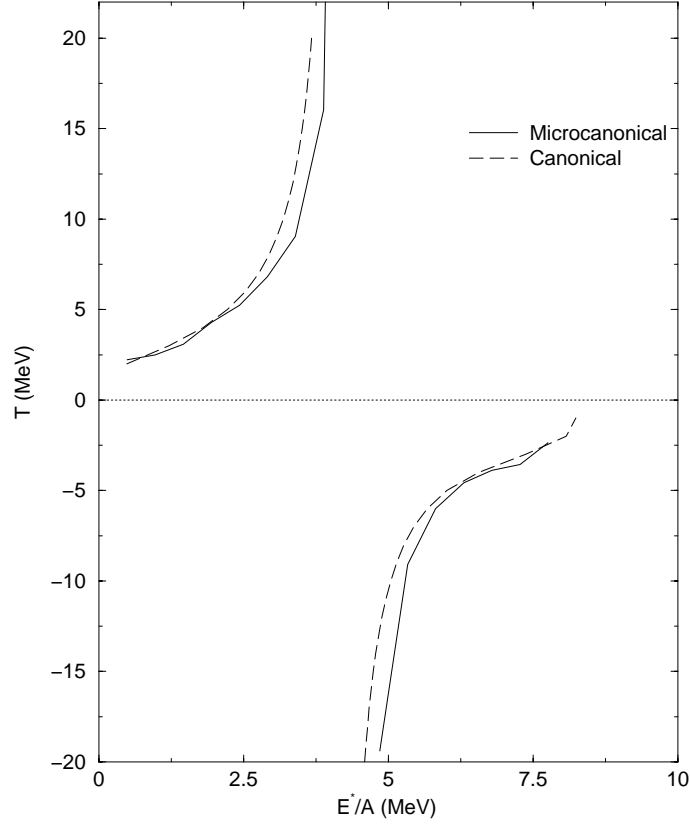


Fig. 2: The caloric curve in SLGM. From Fig. 1 it is clear that the microcanonical definition of temperature would tend to infinity around $E^*/|\epsilon| \approx 8$. For 11 particles this corresponds to about 4 MeV excitation per particle. At higher excitations, the standard definition of temperature leads to large negative temperature. In the canonical calculation, we assume a temperature (positive and negative) and obtain $\langle E^*/A \rangle$ using the table.

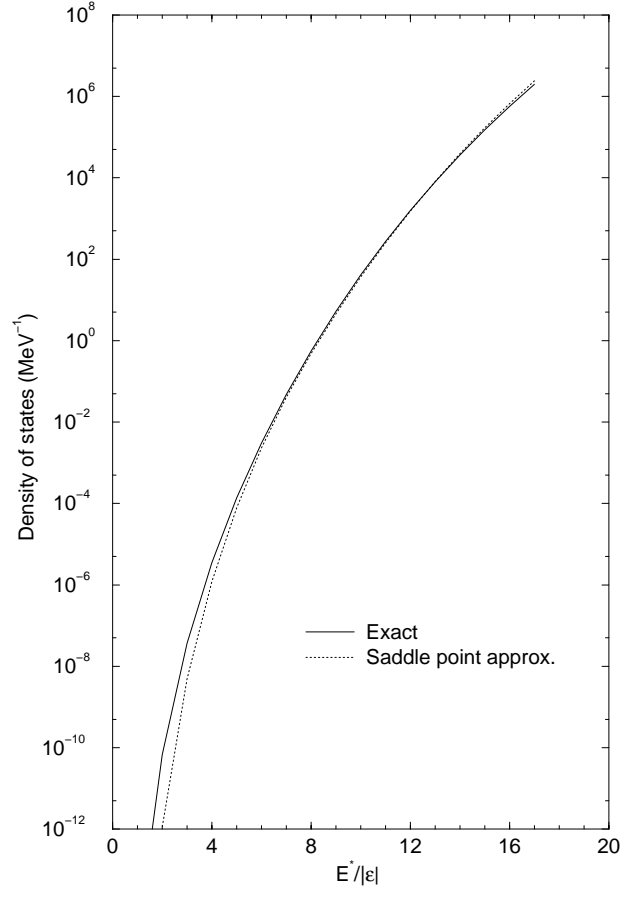


Fig. 3: The density of states in the nuclear LGM. We have plotted (the solid curve) $\sum_i g(E_i^*) \rho_{kin}(E^* - E_i^*)$. For ρ_{kin} we have used eq. (5.1) and multiplied it by $(\frac{V}{h^3})^N$ where $V = \frac{27}{0.16} fm^3$. The dotted curve is the saddle-point approximation for the same density of states. Here $Q(\beta_0)$ is separable into two parts. One part comes from the potential and is directly calculable from the table. This is multiplied by $(2\pi mT)^{3N/2}$ which comes from the kinetic energy.

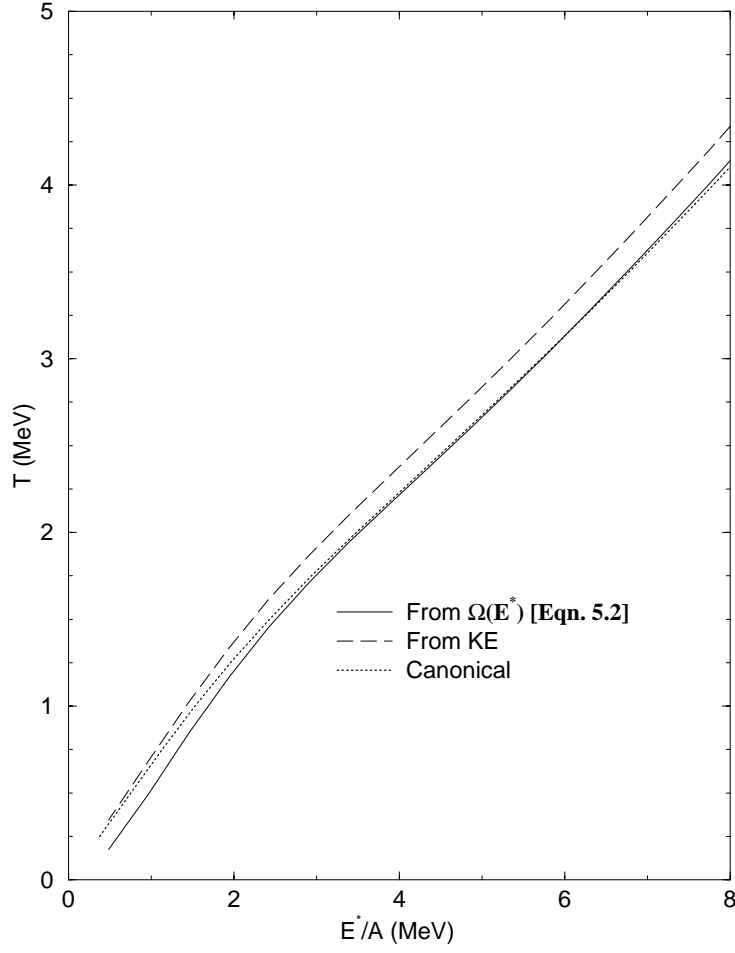


Fig. 4: The caloric curve in microcanonical and canonical treatments. For microcanonical we show two curves. The solid curve takes the log of eq. (5.2) and differentiates with respect to E^* to obtain a temperature. The dashed curve defines T from the average value of kinetic energy (see text). The dotted curve is the canonical caloric curve for the nuclear LGM.

